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OFFICE OF NAVAL RESEARCH

FINAL REPORT

FOR

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NEW THEORETICAL METHODS FOR ELECTRONIC STRUCTURE AND
GAS-PHASE
STATE SPECIFIC OXIDATION/REDUCTION STUDIES

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JANUARY 29, 1992

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The integrated impact of this, my first-ever ONR grant, is detailed in the twenty-four Technical Reports and their associated refereed publications. These Technical Reports are listed on the attached pages. In this Final Report I will briefly discuss only those results which are likely to be of greatest or long-term importance.

A very visible achievement was our successful solution of the world's largest matrix eigenvalue problem - a one billion by one billion configuration interaction eigenvalue problem (Technical Report #7). Prior to our achievement, the largest such problem had been of dimension ca. 75 million. Because these calculations scale on the cube of the matrix dimension, our achievement is quite substantial and has received much attention.

Our work on finding transition states (Technical Report #6 and #8) on potential energy surfaces has had substantial impact; these tools are now incorporated in many ab initio codes such as the GAUSSIAN and GAMESS programs.

The work on so-called Double Rydberg Anions (Technical Report #16) is now reaching maturity and is gaining a reasonable amount of recognition among experimental, physical and inorganic chemists. Although these species were originally (since their discovery in 1987 by K. Bowen and co-workers) thought to be mere novelties, their importance in materials containing their parent cation cores is now believed to be very important.

The work of this group on excited-state potential energy surfaces and reactivity of metal atoms and small main-group clusters (Technical Report #'s 12, 19, 20, 23, and 24) will, I believe, have considerable impact within the next five years. The mechanisms for chemical reaction and electronic-to-vibrational energy flow operative in such prototype species are now of interest to experimental chemists; for these people, our work will be of great help.

Finally, I think that our development and implementation of the so-called Unitary Coupled Electron Pair Approximation (Technical Report #4 and #5) promises to fill an important void in quantum chemistry - the ability to compute electronic energies that are both upper bounds to the true energy and are size-extensive (i.e., scale extensively with the number of electrons in the system). Most commonly used quantum chemical methods possess one or the other of these two attributes, both of which one needs to evaluate intermolecular interaction energies and chemical reaction potential surfaces.

In closing, I wish to express my research group's sincere gratitude to ONR for this financial support. The Ph.D. and postdoctoral associates supported by this grant take seriously our obligation to do the best science possible with the resources available. We look forward to a continued healthy relationship with ONR during the three years of our new grant entitled "Proton and Electron Transfer Reactions (Quantum Treatment Including Intimate Solvent Participation)"

TECHNICAL REPORTS SUBMITTED UNDER

GRANT NOOO14-89-J-1497

NEW THEORETICAL METHODS FOR ELECTRONIC STRUCTURE AND GAS-PHASE
STATE SPECIFIC OXIDATION/REDUCTION STUDIES

Jack Simons, Principal Investigator

<u>Technical Report #</u>	<u>Title and Journal Reference</u>
1	"Application of Cholesky-Like Matrix Decomposition Methods to the Evaluation of Atomic-Orbital Integrals and Integral Derivatives", D. W. O'Neal and J. Simons, Int. J. Quant. Chem. <u>36</u> , 673 (1989).
2	"Modified Rotationally Adiabatic Model for Rotational Autoionization of Dipole-Bound Molecular Anions", Jack Simons, J. Chem. Phys. <u>91</u> , 6858 (1989).
3	" <u>Ab Initio</u> Energy and Structure of H ⁻ (H ₂) ₂ ", R. A. Kendall, J. Simons, M. Gutowski, and G. Chalasinski, J. Phys. Chem. <u>93</u> , 621 (1989).
4	"Size Extensivity Correction of CI Energies Based on Complete Active Space Reference Functions", Jack Simons, Lecture Notes in Chemistry, Vol. <u>50</u> , Springer-Verlag, Berlin, Heidelberg, New York (1988).
5	"A Potentially Size-Consistent Multiconfiguration-Based Coupled Electron Pair Approximation", M. R. Hoffmann and J. Simons, J. Chem. Phys. <u>90</u> , 3671 (1989).
6	"Walking on Potential Energy Surfaces", J. A. Nichols, H. Taylor, P. P. Schmidt and J. Simons, J. Chem. Phys. <u>92</u> , 340 (1990).
7	"Passing the One Billion Limit in Full Configuration Interaction (FCI) Calculations", J. Olsen, P. Jørgensen, J. Simons, Chem. Phys. Lett. <u>169</u> , 463 (1990).
8	"Strategies for Walking on Potential Energy Surfaces Using Local Quadratic Approximations", Jeff Nichols, Jack Simons, Int. J. Quant. Chem. <u>S24</u> , 263 (1990).
9	"Lifetimes of Electronically Metastable Double-Rydberg Anions: FH ₂ ⁻ ", M. Gutowski, J. Simons, J. Chem. Phys. <u>93</u> , 2546 (1990).
10	"Theoretical Study of Anion-Molecule Interactions: H ⁻ HF - H ₂ F ⁻ ", J. A. Nichols, R. A. Kendall, S. J. Cole and J. Simons, J. Phys. Chem., <u>95</u> , 1074 (1991).
11	"First Order Geometrical Response Equations for State Averaged Multiconfigurational Self Consistent Field (SA-MCSCF)

Wavefunctions", K. Bak, J. Boatz, J. Simons, *Inter. J. Quant. Chem.* 40, 361 , (1991).

12 "Electronic Energies, Geometries, and Vibrational Frequencies of the Ground and Low-Lying Excited States of the Boron Trimer", Ramon Hernandez and Jack Simons, *J. Chem. Phys.* 94, 2691 (1991).

13 "A Rigorous Upper Bound Energy for the Unitary Coupled Electron Pair Approximation (CEPA) Method", Jack Simons, *J. Chem. Phys.* 94 , 5252 (1991).

14 "SCF Potential Energy Surfaces for Hydrogen Atom Pairs Within Small Palladium Clusters" J. Anchell, M. Gutowski, J. Nichols, J. Simons, *Int. J. Quant. Chem.* 00 0000 (1992)

15 "An Experimental Chemist's Guide to Ab Initio Quantum Chemistry", Jack Simons, *J. Phys. Chem.* 95, 1017 (1991).

16 "Double-Rydberg Molecular Anions", Jack Simons and Maciej Gutowski, *Chem. Rev.* 91, 669 (1991).

17 "Geometrical Linear Responses and Directional Energy Derivatives for Energetically Degenerate MCSCF Electronic Functions", K L. Bak and J. Simons, *Theor. Chim. Act.*, 00, 0000 (1992).

18 "Ab Initio Quantum Chemistry Study of Formamide - Formamidic Acid Tautomerization", X. Wang, J. Nichols, M. Feyereisen, M. Gutowski, J. Boatz, A.D.J. Haymet, and J. Simons, *J. Phys. Chem.* 95, 10,419 (1991).

19 "Reaction Potential Surface for $B^+(1S) + H_2 \rightleftharpoons HBH^+(1\text{\AA}_g^+), BH^+(2\text{\AA}) + H(2S)$ ", J., Nichols, M. Gutowski, S. J. Cole and J. Simons, *J. Phys. Chem. J. Phys. Chem.* 00, 0000 (1992).

20 "Ab Initio Studies of Ground and Excited Electronic States of MgAr, CdAr, and BeAr" Jerry A. Boatz, Keld Lars Bak, and Jack Simons, *Theoretica Chimica Acta* (accepted for publication)

21 "Direct Atomic-Orbital Based TDHF Calculations of Frequency Dependent Polarizabilities", M. Feyereisen, J. Nichols, J. Oddershede and J. Simons, *J. Chem. Phys.* (accepted for publication).

22 "Relative Stabilities of Fullerene, Cumulene, and Polyacetylene Structures for $C_n:n = 18 - 60$ " M. Feyereisen, M. Gutowski, J. Simons, and J. Almlöf, *J. Chem. Phys.* (accepted for publication)

23 *Ab Initio* Potential Energy Surfaces for $Cd(^1P)_+ H_2 ==> CdH (X ^2\Sigma^+) + H, HCdH (X ^1\Sigma^+), Cd(^3P)_+ H_2$, And $Cd(^1S)_+ H + H^+$ J. Boatz, M. Gutowski, J. Simons, *J. Chem. Phys.* (accepted for publication).

24 "Interactions of the B₃ Cluster with H Atoms and H₂ Molecules" Ramon Hernandez and Jack Simons, *J. Chem. Phys.* (submitted).

**Undergraduate Students, Graduate Students
and Post Doctoral Associates Supported by this Grant**

Mr. John Rusho
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